Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 308 °C

Global applicability domain: Outside

Local applicability domain index: 2.70e-01

Confidence level: 4.21e-01

Nearest Neighbors from the Training Set

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Tris(2-chloroethyl) phosphate
Measured: 330
Predicted: 316

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Sulfonmethane
Measured: 300
Predicted: 295

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1,2-Benzenedicarboxylic acid, bis(2-ethoxyethyl) ester
Measured: 345
Predicted: 323

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Di(2-methoxyethyl) phthalate
Measured: 340
Predicted: 332

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Tetraethyleneglycol dimethacrylate
Measured: 220
Predicted: 252